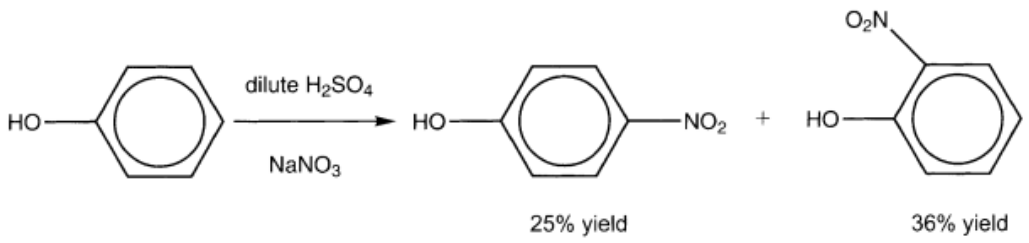
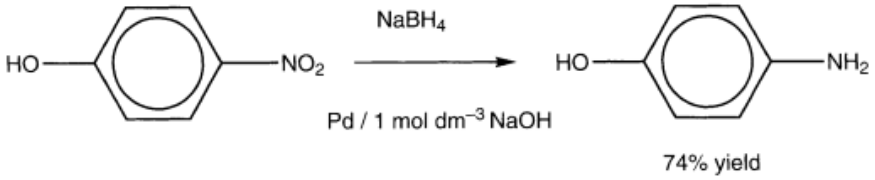
HL Paper 3 Section A Data Response (6) with worked answers

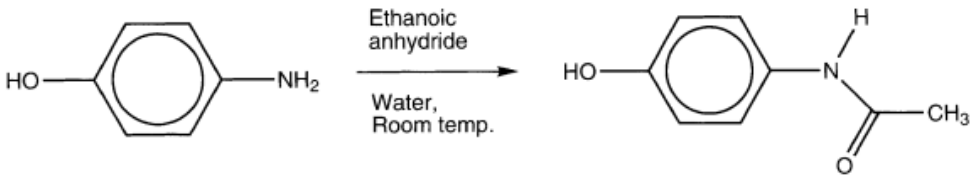
Paracetamol, an over the counter pain-killer, can be synthesised from phenol in three separate steps.



Step 1



Step 2



Step 3

(a) (i) In Step 1 phenol is converted into a mixture of 4-nitrophenol and 2-nitrophenol. Identify the mechanism of this reaction by stating its name. ***[1]***

Electrophilic substitution ***[1]***

(Underlying chemistry concepts can be found in 20.1 Electrophilic substitution.)

(ii) The two products from Step 1 can easily be separated by a process known as steam distillation. Suggest why the boiling point of 2-nitrophenol (216 °C) is considerably lower than the boiling point of 4-nitrophenol (279 °C). ***[2]***

The intermolecular forces responsible for the relatively high boiling points in both 2-nitrophenol and 4-nitrophenol are hydrogen bonding. ***[1]***

The proximity of the $-NO_2$ group to the –OH group in 2-nitrophenol causes some internal hydrogen bonding so the force of attraction between the molecules is less than that between 4-nitrophenol molecules where no internal hydrogen bonding is possible. ***[1]***

(Underlying chemistry concepts can be found in 4.4 Intermolecular forces.)

(b) (i) In Step 2 the 4-nitrophenol is converted into 4-aminophenol. Identify the type of chemical reaction that occurs in this step. ***[1]***

Reduction. ***[1]***

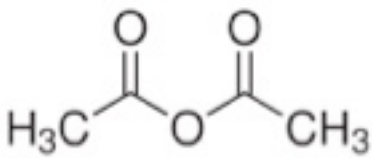
(Underlying chemistry concepts can be found in 20.1 Reduction reactions.)

(II) 4-aminophenol is soluble in aqueous solutions of strong acids.
Deduce the structural formula of the product formed when 4-aminophenol dissolves in dilute hydrochloric acid. ***[1]***

$HO\text{-}C_6H_4\text{-}NH_3^+$ (or $HO\text{-}C_6H_4\text{-}NH_3^+Cl^-$) ***[1]***

(Underlying chemistry concepts can be found in 8.1, 8.2 & 8.4 – Acids and bases.)

(c) The structural formula of ethanoic anhydride is:



(i) Deduce the structural formula of the product, other than paracetamol, formed in Step 3. ***[1]***

CH_3COOH ***[1]***

(Underlying chemistry can be deduced by extending concepts in 10.2 Alcohols.)

(ii) Other than hydroxyl and phenyl, state the name of a functional group present in paracetamol. ***[1]***

Carboxamide ***[1]***
(Amide is not acceptable as this is the class of compound not the functional group)

(Underlying chemistry concepts can be found in 10.1 Fundamentals of organic chemistry.)

(iii) 10.00 g of phenol produced 2.47 g of paracetamol. Assuming the percentage yields of Steps 1 and 2 are as listed, calculate the percentage yield for Step 3. ***[3]***

M_r(phenol, C_6H_6O) = (6 x 12.01) + (6 x 1.01) + 16.00 = 94.12
so amount of phenol in 10.00 g = 10.00 ÷ 94.12 = 1.062×10^{-1} mol ***[1]***

Amount of 4-nitrophenol formed = (25 ÷ 100) x 1.062×10^{-1} = 2.656×10^{-2} mol
Amount of 4-aminophenol formed = (74 ÷ 100) x 2.656×10^{-2} = 1.965×10^{-2} mol
M_r(paracetamol, $C_8H_9NO_2$) = (8 x 12.01) + (9 x 1.01) + 14.00 + (2 x16.00) = 151.17
Amount of paracetamol formed = 2.47 ÷ 151.17 = 1.634×10^{-2} mol ***[1]***

Since 1 mol of 4-aminophenol produces 1 mol of paracetamol
Percentage yield = ((1.634×10^{-2}) ÷ ($1.965 \times 10^{-2)}$) x 100 = 83.2% ***[1]***

(Underlying chemistry concepts can be found in 1.3 Reacting masses and volumes.)